

# The Second Largest Eigenvalue of a Tree\*

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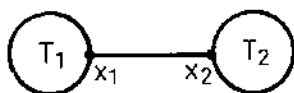
Submitted by N. Biggs

## ABSTRACT

Denote by  $\lambda_2(T)$  the second largest eigenvalue of a tree  $T$ . An easy algorithm is given to decide whether  $\lambda_2(T) \leq \lambda$  for a given number  $\lambda$ , and a structure theorem for trees with  $\lambda_2(T) \leq \lambda$  is proved. Also, it is shown that a tree  $T$  with  $n$  vertices has  $\lambda_2(T) \leq [(n-3)/2]^{1/2}$ ; this bound is best possible for odd  $n$ .

## 1. INTRODUCTION

Suppose that  $T$  is a tree, and  $\lambda$  is a nonnegative real number. In this paper we investigate the question: When is the second largest eigenvalue  $\lambda_2(T)$  of  $T$  smaller than (or equal to)  $\lambda$ ? As basic tool we use the concepts of partial eigenvectors and exitvalues. A partial eigenvector satisfies the eigenvector equation at all vertices but one; the difference at this vertex is given by the exitvalue. The distribution of zeros and signs in the partial eigenvector and the exitvalue is shown to determine the location of  $\lambda$  within the spectrum of  $T$ . Among other things, we derive from this the following structure theorem (cf. Theorem 4.3 below): Let  $T$  be a tree with  $\lambda_2(T) \leq \lambda$ . Then either  $T$  contains a vertex  $x$  such that  $\lambda_1(T - \{x\}) \leq \lambda$ ; or  $T$  is a  $\lambda$ -twin, i.e.,  $T$  has the shape



with subtrees  $T_1$  and  $T_2$  satisfying  $\lambda_1(T_i - \{x_i\}) < \lambda < \lambda_1(T_i)$  for  $i = 1, 2$ . (Here  $\lambda_1$  denotes the largest eigenvalue.) Also, we find an upper bound  $\lambda_2(T)$

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$\leq \sqrt{(n-3)/2}$  on the second largest eigenvalue of a tree with  $n$  vertices, and we determine completely the (infinitely many) trees achieving the bound.

The motivation for the problem considered stems from hyperbolic geometry: The bilinear form associated with a reflection group with Dynkin diagram  $T$  is spherical, affine, or hyperbolic iff  $\lambda_2(T) \leq 2$ . The spherical and affine reflection groups are well known, and Koszul [7] determined the Dynkin diagrams for the minimal hyperbolic reflection groups.

To attack the problem of constructing and classifying other hyperbolic reflection groups, a simple decision algorithm for  $\lambda_2(T) \leq 2$  is needed. This was found tractable for trees and led to the present results. Applications to reflection groups will be reported elsewhere.

## 2. EIGENVALUES

In this section,  $T$  is a connected graph (undirected, without loops or multiple edges). We denote by  $A$  the adjacency matrix of  $T$ , i.e. the matrix  $A = (a_{xy})_{x,y \in T}$  indexed by the vertices of  $T$ , such that  $a_{xy} = 1$  if  $xy$  is an edge, and  $a_{xy} = 0$  otherwise. The characteristic polynomial of  $T$  is denoted by  $P_T(\lambda) = \det(\lambda I - A)$ . We denote the eigenvalues of  $A$ , in decreasing order, by

$$\lambda_1(T) > \lambda_2(T) \geq \dots \geq \lambda_n(T)$$

( $n =$  number of vertices of  $T$ ) and call them the eigenvalues of  $T$  (similarly for eigenvectors). The eigenvalues of the subgraph  $T \setminus \{x\}$  obtained by deleting the vertex  $x \in T$  and the edges containing  $x$  are related to the eigenvalues of  $T$  by the *interlacing property*

$$\lambda_{i+1}(T) \leq \lambda_i(T \setminus \{x\}) \leq \lambda_i(T) \quad (\text{IP})$$

for  $i = 1, \dots, n-1$  (see [2] for a proof).

Let the term  $\lambda$ -eigenvector denote an eigenvector of  $T$  whose corresponding eigenvalue is  $\lambda$ . So  $e$  is a  $\lambda$ -eigenvector (and  $\lambda$  is an eigenvalue) iff  $e$  is nonzero and satisfies the relation

$$\sum_{y \sim x} e_y = \lambda e_x \quad (1)$$

for all  $x \in T$ ; here  $\sim$  means "adjacent." We call a vector  $e$  a *partial*

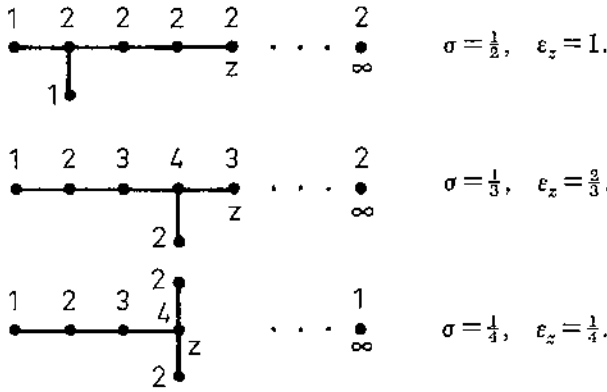
$\lambda$ -eigenvector with respect to a vertex  $z \in T$  if  $e_z = 1$ , and (1) holds for all  $x \in T \setminus \{z\}$ ; in this case the number

$$\varepsilon_{T,z}(\lambda) = \lambda - \sum_{y \sim z} e_y \tag{2}$$

is called a  $\lambda$ -exitvalue of  $T$  with respect to  $z$ . If the  $\lambda$ -exitvalue  $\varepsilon$  is zero, then  $\lambda$  is an eigenvalue of  $T$ , and  $e$  a corresponding eigenvector; if  $\varepsilon$  is nonzero, then it can be thought of as the entry of  $e$  at a hypothetical further vertex  $\infty$  adjacent with  $z$ . For a tree, the equations (1) can be solved recursively by assigning to some end vertex  $x$  the number  $e_x = 1$ ; in this way, one usually gets a multiple of a partial eigenvector.

REMARK. If no confusion is possible, we delete the prefix “ $\lambda$ ” from expressions like “ $\lambda$ -eigenvector” or “ $\lambda$ -exitvalue.”

EXAMPLE. The following diagrams represent some partial eigenvectors and exitvalues for  $\lambda = 2$ . The reader can easily check the relations (1) and (2) for the vector  $e$  whose  $x$ -entry is  $\sigma$  times the label of vertex  $x$ .



For an explanation of the fact that all entries are positive see Theorem 2.4.

THEOREM 2.1. Suppose that the real number  $\lambda$  is not an eigenvalue of  $T - \{z\}$ . Then, with respect to  $z$ , there is a unique partial  $\lambda$ -eigenvector, and

the exitvalue satisfies

$$\varepsilon_{T,z}(\lambda) = \frac{P_T(\lambda)}{P_{T \setminus \{z\}}(\lambda)}. \quad (3)$$

*Proof.* Denote by  $\delta_z = (\delta_{xz})_{x \in T}$  the  $z$ th column of the identity matrix  $I$ , i.e.,  $\delta_z$  is the characteristic vector of  $z$ . Then  $e$  is a partial  $\lambda$ -eigenvector and  $\varepsilon$  the corresponding exitvalue iff  $e$  is a solution of the homogeneous equation

$$(\lambda I - A - \varepsilon \delta_z \delta_z^T) e = 0, \quad (4)$$

with side condition

$$\delta_z^T e = 1. \quad (4a)$$

*Case 1:  $\lambda I - A$  is nonsingular.* Then (4) implies  $e = \varepsilon(\lambda I - A)^{-1} \delta_z$  ( $\delta_z^T e = \varepsilon(\lambda I - A)^{-1} \delta_z^T \delta_z$ ), and (4a) implies that  $\varepsilon^{-1} = \delta_z^T (\lambda I - A)^{-1} \delta_z = P_{T \setminus \{z\}}(\lambda) / P_T(\lambda)$ , by Cramer's rule. Hence  $\varepsilon$  and  $e$  are unique, and in fact these expressions satisfy (4), (4a). Moreover, (3) holds.

*Case 2:  $\lambda I - A$  is singular.* Then  $\lambda$  is an eigenvalue of  $T$ . Let  $e$  be a corresponding eigenvector. If  $e_z = 0$ , then  $e$  is also a  $\lambda$ -eigenvector of  $T \setminus \{z\}$ , contradiction. Hence we may normalize  $e$  so that  $e_z = 1$ ; then  $e$  is a partial eigenvector with exitvalue  $\varepsilon = 0$ , and (3) holds. If  $e'$  is another partial  $\lambda$ -eigenvector, then  $e' - e$  is a  $\lambda$ -eigenvector of  $T \setminus \{z\}$  whence  $e' = e$ . ■

Since the eigenvalues of  $T \setminus \{z\}$  interlace the eigenvalues of  $T$ , (3) implies the following useful results.

**COROLLARY 2.2.** *If  $\lambda$  is an eigenvalue of  $T$  but not of  $T \setminus \{z\}$ , then  $\lambda$  is a simple eigenvalue,  $\varepsilon_{T,z}(\lambda) = 0$ , and the partial  $\lambda$ -eigenvector with respect to  $z \in T$  is the unique  $\lambda$ -eigenvector  $e$  with  $e_z = 1$ .*

**COROLLARY 2.3.** *Between two consecutive eigenvalues of  $T \setminus \{z\}$ , and in the two infinite intervals remaining,  $\varepsilon_{T,z}(\lambda)$  is an increasing function of  $\lambda$  and assumes every value once.*

Partial eigenvectors and exitvalues can be used for the location of eigenvalues of  $T$ . The main tool is the following:

**THEOREM 2.4.** *Suppose that the real number  $\lambda$  is not an eigenvalue of  $T \setminus \{z\}$ . If  $e(z)$  and  $\varepsilon_z$  denote the partial eigenvector and the exitvalue with*

respect to  $z$ , then:

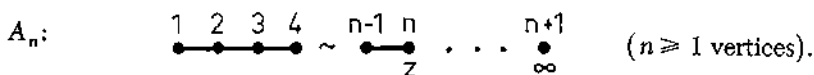
- (i)  $\lambda_1(T) < \lambda$  iff  $e(z) > 0, \epsilon_z > 0$ .
- (ii)  $\lambda_1(T) = \lambda$  iff  $e(z) > 0, \epsilon_z = 0$ .
- (iii)  $\lambda_1(T - \{z\}) < \lambda < \lambda_1(T)$  iff  $e(z) > 0, \epsilon_z < 0$ .

REMARK. Motivated by Theorem 2.4(iii), we call a graph  $T$   $\lambda$ -critical at  $z$  if  $\lambda_1(T - \{z\}) < \lambda < \lambda_1(T)$ .

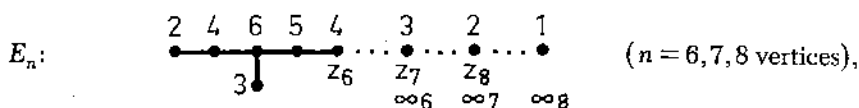
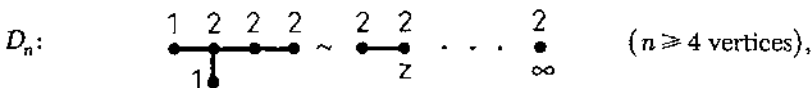
Proof. By (3),  $\epsilon_z = 0$  if  $\lambda_1(T) = \lambda$ , so the statements follow from Corollary 2.3 if we can show that  $e(z) > 0$  iff  $\lambda_1(T - \{z\}) < \lambda$ .

Now (4) holds with  $\epsilon = \epsilon_z, e = e(z)$ ; hence for  $B = A + \epsilon \delta_z \delta_z^T$ , we have  $Be = \lambda e$ , and for any  $s, B + sI$  has the eigenvalue  $\lambda + s$  and corresponding eigenvector  $e$ . But for large  $s, B + sI$  is an irreducible nonnegative matrix. Hence the Frobenius-Perron theory (see e.g. [1]) shows that  $e$  is positive iff  $\lambda$  is the largest eigenvalue of  $B$ . But the proof of Theorem 2.1 shows that  $U - B$  is singular iff  $\epsilon = \epsilon_{T,z}(\epsilon)$ . Hence the eigenvalues of  $B$  are the solutions of  $\epsilon_{T,z}(\epsilon) = \epsilon = \epsilon_{T,z}(\lambda)$ . So, by Corollary 2.3,  $\lambda$  is the largest eigenvalue of  $B$  iff  $\lambda > \lambda_1(T - \{z\})$ . ■

EXAMPLE. We determine all connected graphs  $T$  with largest eigenvalue  $< 2$ . Since a circuit is regular of valency 2, it has eigenvalue 2 and cannot be an induced subgraph of  $T$ . Hence  $T$  is a tree. By Theorem 2.4(i), we have to find all trees with partial 2-eigenvector  $e(z) > 0$  and 2-exitvalue  $\epsilon_z > 0$  for some vertex  $z$ . If  $T$  is a chain, then (up to a scaling factor)  $e(z)$  and  $\epsilon_z$  are given by

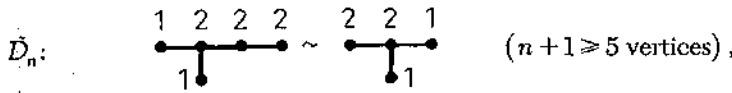


Similarly, we have

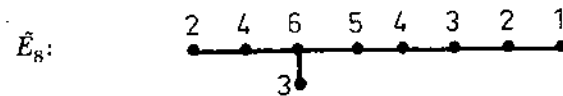
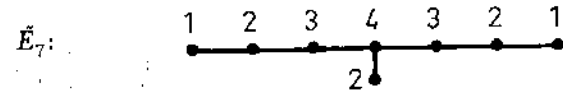
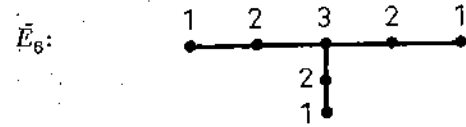


Hence these graphs have  $\lambda_1(T) < 2$ . Now the minimal trees not of type  $A_n$ ,

$D_n$  or  $E_6, E_7, E_8$  are

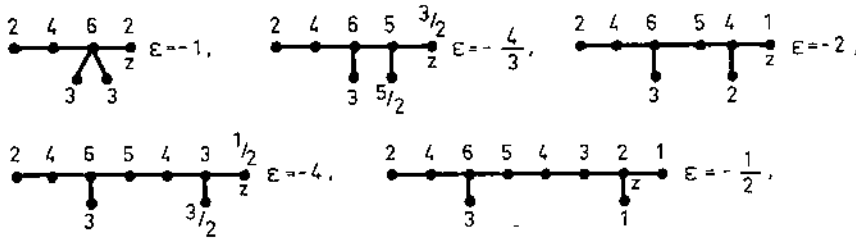


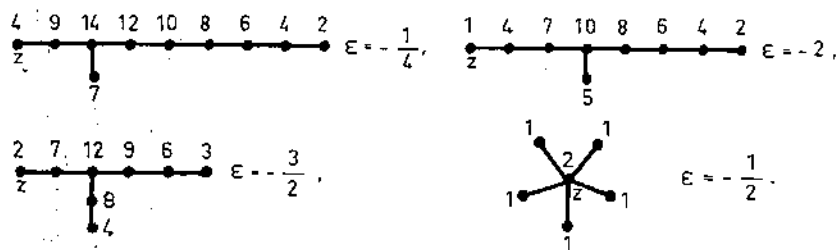
and



The vectors given are eigenvectors, and the exitvalue at any vertex is zero. Hence  $A_n, D_n, E_6, E_7, E_8$  are the only trees with largest eigenvalue  $< 2$ . In fact  $\tilde{D}_n, \tilde{E}_6, \tilde{E}_7,$  and  $\tilde{E}_8$  are the only trees with largest eigenvalue 2 (among the nontrees, only the circuits  $\tilde{A}_n$  occur). The results are all classical.

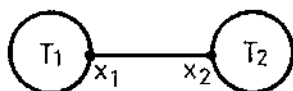
EXAMPLE. In his lectures on hyperbolic coxeter groups, Koszul [7] determined all minimal Dynkin diagrams with  $\lambda_1 > 2$  (Theorems 18-1 and 18-2). We reproduce here those diagrams which are trees without multiple edges. We also give the 2-exitvalue and a multiple of the partial 2-eigenvector with respect to a suitable vector indicated by  $z$ . This is sufficient to check that  $\lambda_1 > 2$ . Minimality and completeness are easily deduced from the previous example.





REMARK. We shall call a graph  $T$  *Euclidean* if  $\lambda_1 \leq 2$ , and *hyperbolic* if  $\lambda_2 \leq 2 < \lambda_1$ . We call  $T$  *spherical* if  $\lambda_1 < 2$ , *affine* or *affine Euclidean* if  $\lambda_1 = 2$ , and *affine hyperbolic* if  $\lambda_2 = 2$ .

Now we consider graphs of shape



which we abbreviate by  $(T_1, x_1, x_2, T_2)$ . Thus the symbol means that  $T_1$  and  $T_2$  are graphs with disjoint vertex sets,  $x_1 \in T_1$ ,  $x_2 \in T_2$ , and  $(T_1, x_1, x_2, T_2)$  is the graph obtained from the disjoint union of  $T_1$  and  $T_2$  by adding the single edge  $x_1 x_2$ . In Section 4 we shall need a special case: We call  $(T_1, x_1, x_2, T_2)$  a  $\lambda$ -*twin* if, for  $i = 1, 2$ ,  $T_i$  is  $\lambda$ -critical at  $x_i$ .

From [2, Theorem 2.12] we have

PROPOSITION 2.5. The characteristic polynomial of  $T = (T_1, x_1, x_2, T_2)$  is

$$P_T(\lambda) = P_{T_1}(\lambda)P_{T_2}(\lambda) - P_{T_1 \setminus \{x_1\}}(\lambda)P_{T_2 \setminus \{x_2\}}(\lambda).$$

As a consequence, we get the following theorem, whose importance will become clear in Section 4.

THEOREM 2.6. Let  $T = (T_1, x_1, x_2, T_2)$  be a  $\lambda$ -twin. For  $i = 1, 2$ , denote by  $\varepsilon_i$  the (negative) exitvalue of  $T_i$  with respect to  $x_i$ . Then:

- (i)  $\lambda_2(T) < \lambda$  iff  $\varepsilon_1 \varepsilon_2 < 1$ .
- (ii)  $\lambda_2(T) = \lambda$  iff  $\varepsilon_1 \varepsilon_2 = 1$ .
- (iii)  $\lambda_2(T) > \lambda$  iff  $\varepsilon_1 \varepsilon_2 > 1$ .

*Proof.* Since  $T_i$  is  $\lambda$ -critical at  $x_i$ , we have  $P_i(t) := P_{T_i \setminus \{x_i\}}(t) > 0$  for all  $t \geq \lambda$ . In particular, the exitvalues  $\varepsilon_i(t) := \varepsilon_{T_i, x_i}(t)$  are defined. Now by Theorem 2.1 and Proposition 2.5,

$$P_T(t) = [\varepsilon_1(t)\varepsilon_2(t) - 1] P_1(t)P_2(t). \quad (5)$$

Put  $\lambda_1 = \lambda_1(T)$ ,  $\lambda_2 = \lambda_2(T)$ , and denote by  $\lambda_3$  the largest eigenvalue of  $T$  strictly smaller than  $\lambda_2$ . Then  $P_T(t)$  is negative for  $\lambda_2 < t < \lambda_1$ , zero for  $t = \lambda_2$ , and positive for  $\lambda_3 < t < \lambda_2$ . On the other hand,  $T_1$  and  $T_2$  are  $\lambda$ -critical at  $x_1$  and  $x_2$ , respectively, whence  $T \setminus \{x_1\}$  has largest eigenvalue  $> \lambda$ , and  $T \setminus \{x_1, x_2\}$  has largest eigenvalue  $< \lambda$ . So, by interlacing,  $\lambda_3 < \lambda < \lambda_1$ , and we get the result by putting  $t = \lambda$  into (5). ■

We also have some information on the eigenvectors of  $(T_1, x_1, x_2, T_2)$ , not necessarily a twin.

**PROPOSITION 2.7.** *Let  $T = (T_1, x_1, x_2, T_2)$ , and let the real number  $\lambda$  be not an eigenvalue of  $T_1 \setminus \{x_1\}$  or  $T_2 \setminus \{x_2\}$ . For  $i = 1, 2$ , denote by  $e^{(i)}$  and  $\varepsilon_i$  the partial eigenvector and the exitvalue of  $T_i$  with respect to  $x_i$ . Then  $\lambda$  is an eigenvalue of  $T$  iff  $\varepsilon_1\varepsilon_2 = 1$ ; in this case, every  $\lambda$ -eigenvector has the form*

$$e = \begin{pmatrix} s_1 e^{(1)} \\ s_2 e^{(2)} \end{pmatrix}, \quad s_2 = s_1 \varepsilon_1, \quad s_1 = s_2 \varepsilon_2; \quad (6)$$

in particular,  $\lambda$  is a simple eigenvalue of  $T$ .

*Proof.* Suppose that  $\lambda$  is an eigenvalue of  $T$ , and  $e$  a  $\lambda$ -eigenvector. The numbers  $s_i = e_{x_i}$  are nonzero, since otherwise  $T_i \setminus \{x_i\}$  would have an eigenvalue  $\lambda$  corresponding to the restriction of  $e$  to  $T_i \setminus \{x_i\}$ . Hence we can write the restriction of  $e$  to  $T_i$  in the form  $s_i \bar{e}^{(i)}$ , and  $\bar{e}^{(i)}$  is easily seen to be the (unique) partial eigenvector  $e^{(i)}$  of  $T_i$ . Moreover, the relations (1) for  $x = x_1$  and  $x = x_2$  give  $s_2 = s_1 \varepsilon_1$ ,  $s_1 = s_2 \varepsilon_2$ ; in particular  $\varepsilon_1 \varepsilon_2 = 1$ . Conversely, if  $\varepsilon_1 \varepsilon_2 = 1$ , then (6) defines an eigenvector of  $T$ . ■

### 3. SPECIAL VERTICES OF A TREE

From now on,  $T$  is a tree. In this section we prove some results about the possible zero entries of an eigenvector of  $T$ . Call a vertex  $x \in T$   $\lambda$ -essential if



there is a  $\lambda$ -eigenvector  $e$  with  $e_x \neq 0$ ,  $\lambda$ -special if it is not essential, but adjacent with some essential point, and  $\lambda$ -inessential otherwise. Call a tree  $T$   $\lambda$ -primitive if  $\lambda$  is an eigenvalue of  $T$  and all vertices are  $\lambda$ -essential.

A subtree  $T_1$  of  $T$  is called *extremal* if, for some vertex  $x \in T$ ,  $T_1$  is a component of  $T \setminus \{x\}$ ; equivalently, if the graph  $T_2 = T \setminus T_1$  (obtained by deleting the vertices of  $T_1$ ) is nonempty and connected, hence also a tree. Note that in this case,  $T_1$  and  $T_2$  are connected by a unique edge  $x_1x_2$  with  $x_1 \in T_1$ ,  $x_2 \in T_2$ , and  $T = (T_1, x_1, x_2, T_2)$ .

**THEOREM 3.1.** *A tree  $T$  is  $\lambda$ -primitive iff  $T$ , but no extremal subtree of  $T$ , has eigenvalue  $\lambda$ .*

*Proof.* Let  $T$  be a tree with eigenvalue  $\lambda$ , and let  $e$  be a  $\lambda$ -eigenvector. If  $e_x = 0$  for some  $x \in T$ , then the relations (I) show that each component of  $T \setminus \{x\}$  which contains a vertex  $y$  with  $e_y \neq 0$  is an extremal subtree with eigenvalue  $\lambda$ . Hence if  $T$  contains no extremal subtree with eigenvalue  $\lambda$ , then  $T$  is  $\lambda$ -primitive.

Conversely, if  $T$  contains extremal subtrees with eigenvalue  $\lambda$ , then let  $T_1$  be minimal (with respect to inclusion) among these. Denote the tree  $T \setminus T_1$  by  $T_2$ , so that  $T = (T_1, x_1, x_2, T_2)$  for certain  $x_1 \in T_1$ ,  $x_2 \in T_2$ . Since  $T_1$  is minimal,  $\lambda$  is not an eigenvalue of  $T_1 \setminus \{x_1\}$ . Now the restriction  $e^{(1)}$  of  $e$  to  $T_1$  is a multiple of the partial eigenvector of  $T_1$  with respect to  $x_1$  (by Proposition 2.7), and by Corollary 2.2,  $e^{(1)}$  is in fact a  $\lambda$ -eigenvector of  $T_1$ . Hence by (I),  $e_{x_2} = 0$ . Since this holds for every  $\lambda$ -eigenvector  $e$ ,  $x_2$  is not  $\lambda$ -essential, and so  $T$  is not  $\lambda$ -primitive. ■

**COROLLARY 3.2.** *If  $\lambda$  is a multiple eigenvalue of a tree  $T$ , then  $T$  contains a  $\lambda$ -special point.*

*Proof.* For any  $x \in T$ ,  $T \setminus \{x\}$  still has  $\lambda$  as an eigenvalue; hence some component of  $T \setminus \{x\}$ , which is an extremal tree, has  $\lambda$  as an eigenvalue. By Theorem 3.1,  $T$  is not primitive and hence contains a special point. ■

**COROLLARY 3.3.** *A  $\lambda$ -primitive tree has  $\lambda$  as a simple eigenvalue, and the corresponding eigenvector has no zero entries.*

**THEOREM 3.4.** *Let  $T$  be a tree with  $f$ -fold eigenvalue  $\lambda$ ,  $f \geq 1$ . Then:*

- (i) *If  $x$  is an essential vertex then  $\lambda$  is an  $(f - 1)$ -fold eigenvalue of  $T \setminus \{x\}$ .*
- (ii) *If  $x$  is an inessential vertex, then  $\lambda$  is an  $f$ -fold eigenvalue of  $T \setminus \{x\}$ .*

(iii) If  $x$  is a special vertex, then  $\lambda$  is an  $(f+1)$ -fold eigenvalue of  $T \setminus \{x\}$ ; moreover,  $x$  is adjacent to at least two essential vertices.

*Proof.* (i): In [5], it is shown that  $P(T \setminus \{x\}, t)/P(T, t)$ , considered as a function in  $t$ , has simple poles just at those eigenvalues  $\lambda$  of  $T$  for which there is some  $\lambda$ -eigenvector  $e$  with  $e_x \neq 0$  (see Theorem 5.2 of [5], and its proof). Hence  $\lambda$  is an  $(f-1)$ -fold eigenvalue of  $T \setminus \{x\}$  iff  $x$  is  $\lambda$ -essential.

(ii) and (iii): If  $x$  is not essential, then an eigenvector  $e$  of  $T$  is also an eigenvector of  $T \setminus \{x\}$ . If  $x$  is inessential, then the converse also holds, so  $T \setminus \{x\}$  has  $\lambda$  as an  $f$ -fold eigenvalue. But if  $x$  is special, then one extra relation  $\sum_{y \sim x} e_y = 0$  has to be satisfied. So the eigenspace of  $T \setminus \{x\}$  for  $\lambda$  must have one dimension more, i.e.,  $\lambda$  is an  $(f+1)$ -fold eigenvalue of  $T \setminus \{x\}$ . If  $x$  were only adjacent with one essential point  $y$ , then the relation would reduce to  $e_y = 0$ , contradicting the fact that  $y$  is essential. ■

**COROLLARY 3.5.** *Let  $T$  be a tree with  $f$ -fold eigenvalue  $\lambda$ ,  $f \geq 1$ . Denote by  $E$  the forest induced on the essential vertices. Then every component of  $E$  has  $\lambda$  as a simple eigenvalue. Moreover,  $f$  equals the number of components of  $E$  minus the number of special vertices of  $T$ .*

*Proof.* For each  $x \in E$ , some eigenvector  $e$  of  $T$  has  $e_x \neq 0$ . Each such  $e$  is also an eigenvector of  $E$ , and hence of the component of  $E$  containing  $x$ . So every component of  $E$  is  $\lambda$ -primitive, and by Corollary 3.3, has  $\lambda$  as a simple eigenvalue. From this, and the preceding theorem, the second part follows. ■

**EXAMPLE.** Take  $\lambda = 0$ . By Theorem 3.1, a 0-primitive tree consists of a single vertex, since every end vertex is an extremal subtree with eigenvalue  $\lambda = 0$ . In particular, for an arbitrary tree,  $E$  is a coclique. The 0-special vertices are closely related to  $k$ -matchings (sets of  $k$  disjoint edges) of  $T$ . In fact, following some remarks by Godsil (private communication), we have

**PROPOSITION 3.6.** *Let  $T$  be a tree with  $n$  vertices, and let  $k$  be the maximal size of a matching. Then:*

- (i) 0 is an  $(n - 2k)$ -fold eigenvalue of  $T$ .
- (ii) No vertex is 0-inessential.
- (iii) A vertex is 0-special iff it is common to all  $k$ -matchings.
- (iv) An edge contains one or two 0-special vertices.
- (v) There are exactly  $k$  0-special vertices, and every edge of a  $k$ -matching contains a unique 0-special vertex.

*Proof.* (i) is well known; see e.g. Proposition 1.1 of [2].

If  $x \in T$  is not common to all  $k$ -matchings then the maximal size of a matching of  $T \setminus \{x\}$  is  $k$ , whence 0 is an  $(n-1-2k)$ -fold eigenvalue of  $T \setminus \{x\}$  [apply (i) to  $T \setminus \{x\}$ ]. Hence  $x$  is 0-essential (Theorem 3.4). On the other hand, if  $x \in T$  is common to all  $k$ -matchings, then the maximal size of a matching of  $T \setminus \{x\}$  is  $k-1$ , 0 is an  $(n+1-2k)$ -fold eigenvalue of  $T \setminus \{x\}$ , and  $x$  is 0-special. This proves (ii) and (iii). Since  $E$ , the set of 0-essential vertices, is a coclique, (iv) holds.

Finally, denote by  $e$  and  $s$  the numbers of 0-essential and 0-special vertices, respectively.  $E$  is an  $e$ -coclique; hence by (i) and Corollary 3.5, the multiplicity of 0 is  $n-2k=e-s$ . But  $n=e+s$ , whence  $s=k$ ; i.e.,  $T$  contains  $k$  0-special vertices. On each edge of a  $k$ -matching there is at least one, and hence exactly one, of these vertices. ■

#### 4. THE SECOND LARGEST EIGENVALUE OF A TREE

Here we investigate the structure of trees with  $\lambda_2(T) \leq \lambda$ . Let us call a tree  $T$   $\lambda$ -trivial if there is a vertex  $x \in T$  such that  $\lambda_1(T - \{x\}) \leq \lambda$  — equivalently, if all components of  $T \setminus \{x\}$  are trees with largest eigenvalue  $\leq \lambda$ . Because the eigenvalues of  $T \setminus \{x\}$  interlace those of  $T$ , a  $\lambda$ -trivial tree has  $\lambda_2(T) \leq \lambda$ . It is easy to find sufficient conditions for  $\lambda$ -triviality:

**PROPOSITION 4.1.** *If a tree  $T$  with  $\lambda_2(T) \leq \lambda$  contains extremal subtrees with eigenvalue  $\lambda$ , then  $T$  is  $\lambda$ -trivial.*

*Proof.* Let  $T_0$  be an extremal subtree of  $T$  with eigenvalue  $\lambda$ , and let  $x$  be the vertex such that  $T_0$  is a component of  $T \setminus \{x\}$ . Since the eigenvalues of  $T \setminus \{x\}$  interlace those of  $T$ ,  $T \setminus \{x\}$  has exactly one eigenvalue  $> \lambda_2(T)$ , which must be  $\lambda$ ; the other eigenvalues are  $\leq \lambda_2(T) \leq \lambda$ . Hence  $T$  is  $\lambda$ -trivial. ■

Using Theorem 3.1 and Corollary 3.2, we immediately obtain

**COROLLARY 4.2.** *If  $\lambda_2(T)$  is a multiple eigenvalue of a tree  $T$ , then  $T$  is  $\lambda_2$ -trivial.*

We are now able to prove our main result. Together with Theorem 2.6, it characterizes all trees with  $\lambda_2(T) \leq \lambda$ .

**THEOREM 4.3.** *A tree  $T$  with  $\lambda_2(T) \leq \lambda$  is either  $\lambda$ -trivial or a  $\lambda$ -twin.*

*Proof.* Suppose that  $T$  is not  $\lambda$ -trivial. By Proposition 4.1,  $T$  contains no extremal subtree with eigenvalue  $\lambda$ . But there are extremal subtrees with largest eigenvalue  $> \lambda$ , since for all  $x \in T$ ,  $\lambda_1(T \setminus \{x\}) > \lambda$ . Let  $T_1$  be an extremal subtree, minimal with respect to the property  $\lambda_1(T_1) > \lambda$ . With  $T_2 = T \setminus T_1$ ,  $T$  can be written as  $T = (T_1, x_1, x_2, T_2)$ . By minimality of  $T_1$ ,  $\lambda_1(T_1 \setminus \{x_1\}) \leq \lambda$ , and hence  $< \lambda$ ; so  $T_1$  is critical at  $x_1$ .

Now  $T$  is not  $\lambda$ -trivial; hence  $T \setminus \{x_1\}$  has an eigenvalue  $> \lambda$ , and so  $\lambda_1(T_2) > \lambda$ . By construction,  $\lambda_1(T_1) > \lambda \geq \lambda_2(T)$ . Since  $T \setminus \{x_2\}$  is the disjoint union of  $T_1$  and  $T_2 \setminus \{x_2\}$ ,  $\lambda_1(T_1)$  is an eigenvalue  $\geq \lambda_2(T)$  of  $T \setminus \{x_2\}$ . By interlacing, the other eigenvalues of  $T \setminus \{x_2\}$  are  $\leq \lambda_2(T) \leq \lambda$ . In particular, the eigenvalues of  $T_2 \setminus \{x_2\}$  are  $\leq \lambda$ , and hence even  $< \lambda$ . Therefore  $T_2$  is critical at  $x_2$ , and  $T$  is a twin. ■

**REMARK.** It is easy to see that a  $\lambda$ -twin cannot be  $\lambda$ -trivial, and that a tree can be written in at most one way as a  $\lambda$ -twin.

In Theorem 2.6, we showed how to decide whether a  $\lambda$ -twin  $T$  has  $\lambda_2(T) < \lambda$  or  $\lambda_2(T) = \lambda$ ; the next result complements this by a criterion for  $\lambda_2(T) = \lambda$  for  $\lambda$ -trivial trees. Note that  $\lambda_2(T) < \lambda$  if this criterion fails.

**THEOREM 4.4.** *Let  $T$  be a  $\lambda$ -trivial tree, and  $x \in T$  a vertex with  $\lambda_1(T \setminus \{x\}) \leq \lambda$ . Then  $\lambda_2(T) = \lambda$  iff  $f+1 \geq 2$  components of  $T \setminus \{x\}$  have (largest) eigenvalue  $\lambda$ ; in this case,  $x$  is a special vertex of  $T$ , and  $\lambda$  is an  $f$ -fold eigenvalue of  $T$ .*

*Proof.* A 0-trivial tree is a star, and the statement is obvious. Hence assume that  $\lambda \neq 0$ . Suppose that  $\lambda_2(T) = \lambda$ , and let  $e$  be a  $\lambda$ -eigenvector of  $T$ . Denote by  $T'$  the tree induced on the set consisting of  $x$  and those components of  $T \setminus \{x\}$  which have some nonzero entry in  $e$ . Suppose first that  $T' \setminus \{x\}$  contains a component  $T_0$  with largest eigenvalue  $\lambda$ ; let  $x_0$  be the vertex in  $T_0$  adjacent to  $x$ . If  $e_{x_0} = 0$ , then the restriction of  $e$  to  $T_0 \setminus \{x_0\}$  is a  $\lambda$ -eigenvector of  $T_0 \setminus \{x_0\}$  (nonzero by construction of  $T'$ ). But  $\lambda_1(T_0 \setminus \{x_0\}) < \lambda_1(T_0) = \lambda$ , contradiction. Hence  $e_{x_0} \neq 0$ , and  $e$  can be normalized so that  $e_{x_0} = 1$ . Then the restriction of  $e$  to  $T_0$  is a partial eigenvector of  $T_0$ , and by Theorem 2.2, it is an eigenvector. Therefore, the relations (1) for  $x = x_0$  imply  $e_x = 0$ . This holds for every  $\lambda$ -eigenvector  $e$  of  $T$ ; so  $x$  is special. Now apply Theorem 3.4(iii) to get the desired result.

Next suppose that  $T' \setminus \{x\}$  has no component with largest eigenvalue  $\lambda$ . Then  $e_x \neq 0$ , since otherwise  $e$  is a  $\lambda$ -eigenvector of  $T' \setminus \{x\}$ , and  $\lambda_1(T' \setminus \{x\}) < \lambda$ . Since  $\lambda \neq 0$ , some neighbor  $x_1$  of  $x$  must have  $e_{x_1} \neq 0$  [by (1)]. Write  $x_2 = x$ , write  $T_1$  for the component of  $T' \setminus \{x_2\}$  containing  $x_1$ , and  $T_2$  for the component of  $T' \setminus \{x_1\}$  containing  $x_2$ . Then  $T' = (T_1, x_1, x_2, T_2)$ , and  $\lambda_1(T_1) <$

$\lambda, \lambda_1(T_2 \setminus \{x_2\}) < \lambda$ . Denote by  $e^{(i)}$  and  $\varepsilon_i$  the partial eigenvector and exitvalue of  $T_i$  with respect to  $x_i$ . Then by Theorem 2.4,  $e^{(1)} > 0, \varepsilon_1 > 0, e^{(2)} > 0$ , and by Proposition 2.7,  $e$  or  $-e$  is positive on  $T'$ , hence nonnegative on  $T$ . But this implies (Perron-Frobenius) that  $\lambda = \lambda_1(T) > \lambda_2(T)$ , a contradiction.

The converse follows again from Theorem 3.4(iii). ■

The theorems just proved have an interesting corollary. Let  $e$  be a  $\lambda$ -eigenvector of a tree  $T$ . We say that an edge  $xy$  of  $T$  is a *sign change* of  $e$  if  $e_x e_y < 0$ . From our Theorems 4.3 and 4.4, and Theorems 2.4(iii) and 2.6(ii), we find:

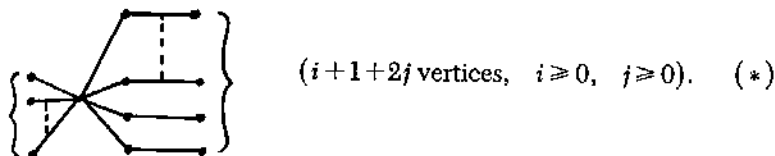
**COROLLARY 4.4a.** *Let  $e$  be an eigenvector for the second largest eigenvalue of a tree. If all entries of  $e$  are nonzero, then  $e$  has exactly one sign change.*

This is a special case of the following theorem [6]:

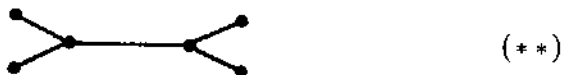
**THEOREM 4.5 (Godsil).** *Let  $e$  be an eigenvector for the eigenvalue  $\lambda_i(T)$  of a tree. If all entries of  $e$  are nonzero, then  $e$  has exactly  $i - 1$  sign changes.*

Note that the special case  $i = 1$  (no sign change) of Theorem 4.5 is a consequence of Perron-Frobenius theory. Also, the case where  $T$  is a path is a special case of a result of Gantmacher and Krein [4] on oscillation matrices (their Satz 6 in Kap. II, §5).

**EXAMPLE.** We determine the trees with  $\lambda_2 \leq 1$ . It is obvious that a tree with largest eigenvalue  $< 1$  is a single vertex, and a tree with largest eigenvalue  $= 1$  is a single edge. Hence the 1-trivial graphs are of the shape



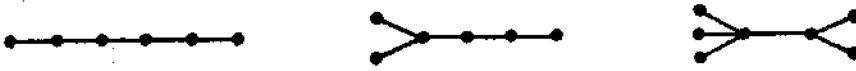
Also, if a tree  $T$  is 1-critical at  $x$ , then  $T \setminus \{x\}$  is a coclique of size  $s \geq 2$ , say, and the exitvalue is  $\varepsilon = 1 - s \leq -1$ . Hence the only way to get a 1-twin with  $\varepsilon_1 \varepsilon_2 \leq 1$  is to take  $s_1 = s_2 = 2$ ; by Theorem 2.6, the only twin with  $\lambda_2 \leq \lambda$  is



Hence we have:

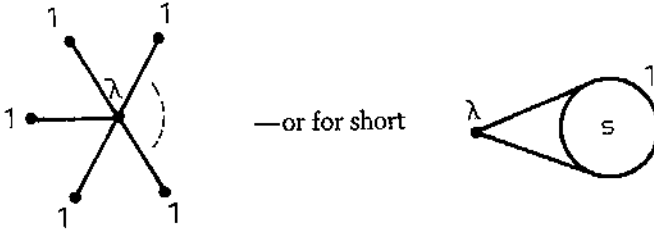
**THEOREM 4.6.** *A tree with  $\lambda_2 \leq 1$  either is of shape (\*), or is the graph (\*\*).*

**REMARK.** A different proof can be given by forbidden subtrees. In fact, by the tables in [2], the second largest eigenvalues of the trees

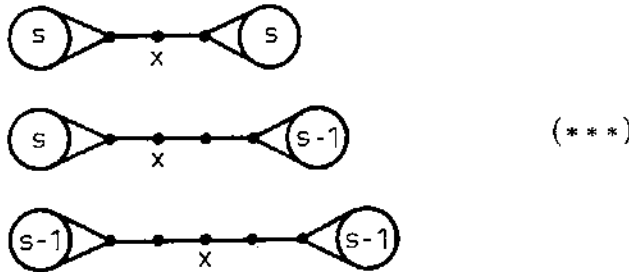


are  $> 1$ , and the trees (\*), (\*\*) are the only trees with no such induced subtree.

**EXAMPLE.** A star with  $n = s + 1$  vertices,



—has largest eigenvalue  $\sqrt{s} = \sqrt{n-1}$ , since the indicated vector is a positive eigenvector for  $\lambda = \sqrt{s}$ . Hence a tree  $T$  with a vertex  $x$  such that  $T \setminus \{x\}$  is a disjoint union of  $m$  stars with  $s+1$  vertices is  $\sqrt{s}$ -trivial; hence  $\lambda_2 \leq \sqrt{s}$ . If  $m \geq 2$ , then by Theorem 4.4,  $\lambda_2 = \sqrt{s}$  is an  $(m-1)$ -fold eigenvalue of  $T$ . In particular, the three trees



have  $n = 2s + 3$  vertices and  $\lambda_2 = \sqrt{s} = \sqrt{(n-3)/2}$  (in particular, there are trees with arbitrarily large  $\lambda_2$ ). The trees (\*\*\*) are extremal in the following sense:

**THEOREM 4.7:** *Let  $T$  be a tree with  $n$  vertices. Then*

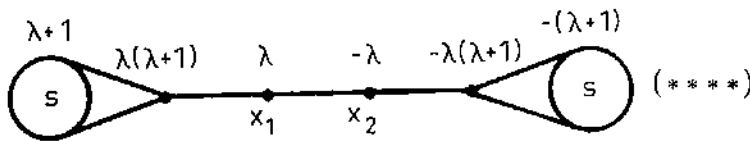
- (i)  $\lambda_1(T) \leq \sqrt{n-1}$ , with equality iff  $T$  is a star;
- (ii)  $\lambda_2(T) \leq \sqrt{(n-3)/2}$ , with equality iff  $T$  is one of the trees (\*\*\*) .

*Proof.* (i):  $T$  is bipartite; hence with  $\lambda_1$ , also  $-\lambda_1$  is an eigenvalue of  $T$ . Therefore,  $2\lambda_1^2 \leq \sum \lambda_i^2 = \text{tr } A^2 = 2 \times (\text{number of edges of } T) = 2(n-1)$ , and so  $\lambda_1 \leq \sqrt{n-1}$ . If equality holds, then  $\lambda_2 = \dots = \lambda_{n-1} = 0$ ,  $\lambda_n = -\lambda_1$ . Hence  $A$  has rank 2. Since  $T$  is bipartite, this implies that  $T$  is complete bipartite, and since  $T$  is a tree, it must be a star.

(ii): There is a vertex  $x \in T$  such that all components of  $T \setminus \{x\}$  have size  $\leq (n-1)/2$ . For if  $T \setminus \{x_1\}$  has a component  $T_0$  of size  $\geq n/2$ , then the remaining components have size  $< n/2 - 1$  together; thus if  $x_2$  is the neighbor of  $x_1$  in  $T_0$  then in  $T \setminus \{x_2\}$ , the component of  $x_1$  has size  $< n/2$  and hence  $\leq (n-1)/2$ , and the other components of  $T \setminus \{x_2\}$  are contained in  $T_0 \setminus \{x_2\}$  and hence have size less than the size of  $T_0$ . If we repeat this process, we obtain after a finite number of steps an  $x$  with the required property.

Now, by interlacing,  $\lambda_2(T) \leq \lambda_1(T \setminus \{x\}) \leq \sqrt{(n-3)/2}$  by (i), and equality implies that some component  $T_1$  of  $T \setminus \{x\}$  has size  $(n-1)/2$  and is a star. But then  $T_1$  is an extremal subtree with eigenvalue  $\sqrt{(n-3)/2} = \lambda_2$ , and by Theorem 4.4,  $T \setminus \{x\}$  has another component  $T_2$  with eigenvalue  $\lambda_2$ , which again must be a star of size  $(n-1)/2$ . Now we already have all vertices, and the only ways of getting a tree are those shown in (\*\*\*) . ■

**REMARK.** In particular, for a tree with an even number  $n$  of vertices,  $\lambda_2(T) < \sqrt{(n-3)/2}$ . Probably the unique extremal trees in this case are

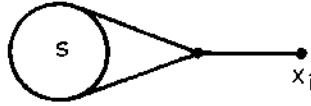


with  $n = 2s + 4$  vertices; this can be verified for  $n \leq 10$  by the tables in [2]. The second largest eigenvalue of (\*\*\*) is the positive root  $\lambda$  of the

equation

$$\lambda^3 + \lambda^2 - (s+1)\lambda - s = 0,$$

as can be seen from the indicated eigenvector. Since  $s = \lambda^2 - \lambda / (\lambda + 1) < \lambda^2 < \lambda^2 + 1 / (\lambda + 1) = s + 1$ , it follows that



is  $\lambda$ -critical, and both exitvalues are  $\varepsilon_1 = \varepsilon_2 = -1$ . So we have a twin with  $\varepsilon_1 \varepsilon_2 = 1$  (cf. Proposition 2.7). (It is also seen that there is exactly one sign change.)

We end this section with explicit recursive formulas for the computation of partial eigenvectors and exitvalues of a tree. Let  $T$  be a tree, and  $z \in T$ . Denote the neighbors of  $z$  by  $z_1, \dots, z_s$ . Then the components of  $T \setminus \{z\}$  can be labeled as  $T_1, \dots, T_s$  in such a way that  $z_i \in T_i$  for  $i = 1, \dots, s$ . Let  $e_i$  and  $\varepsilon_i$  be the partial eigenvector and exitvalue of  $T_i$  with respect to  $z_i$ . If all  $\varepsilon_i$  are nonzero, then the partial eigenvector  $e$  of  $T$  has  $e_z = 1$ , and agrees on  $T_i$  with  $\varepsilon_i^{-1} e^{(i)}$  [by the relations (1)], and so is determined. Also, the exitvalue  $\varepsilon$  of  $T$  with respect to  $z$  is given by the formula

$$\varepsilon = \lambda - \sum_i \varepsilon_i^{-1}.$$

These remarks can be used to find a partial eigenvector and/or an exitvalue recursively. The process breaks down if some  $\varepsilon_i$  becomes zero. But then  $T_i$  is an extremal subgraph with eigenvalue  $\lambda$ ; so this breakdown cannot occur in the range  $\lambda > \lambda_1(T \setminus \{z\})$ .

Note that in actual computation it may be more convenient to compute a multiple of the partial eigenvector, and normalize at the end of the computation.

REMARK. After submission of the manuscript, I learnt that Godsil's Theorem 4.5 is a particular case of a theorem of Fiedler [3], and that a paper by Maxwell [8] contains the case  $\lambda_2(T) \neq \lambda$  of my Theorem 4.3. I want to thank Jürgen Garloff and Barry Monson for calling my attention to these papers.

*I want to thank Chris Godsil for valuable suggestions which improved Section 3.*



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